Geometry of N-particle clusters in two-dimensions: Some exact results

G. Date and M. V. N. Murthy
The Institute of Mathematical Sciences, Madras 600 113, India.
(February 1, 2008)

We report on a study of a finite system of classical confined particles in two-dimensions in the presence of a uniform magnetic field and interacting via a two-body repulsive potential. We develop a simple analytical method of analysis to obtain ground state energies and configurations. We prove analytically the minimum energy configurations are independent of the nature of two body interaction and the magnetic field. In particular we prove that the first transition from a single shell occurs when the number of particles changes from five to six. These results are exact.

PACS numbers: 02.60.Cb, 71.10.-w

There has been considerable progress in recent years in the study of electrons in quasi-two-dimensional systems both experimentally and theoretically [1]. There are several examples of these systems but the most important one from our point of view is that of electrons in a quantum dot. There have been several studies on the ordering and transitions of charged particles in two-dimensions [2–6]. In a recent Monte Carlo study, Bedanov and Peeters [5](see also Bolten and Rossler [6]) have analysed the classical ground state of a system of confined charged particles interacting through Coulomb interaction. By minimising the classical energy, they obtain numerically the shell structure in a cluster of N-particles. They have systematically listed the shell structure in a "Mendeleev" table for $N \leq 52$, and for a few large clusters. Similar results are available also for logarithmic two-body interaction [2].

In this paper we consider such a cluster in which the repulsive two-body potential is either a power-law(or logarithmic). We devise a simple analytical method to obtain the classical ground state energy in *two* steps. First we minimise the energy for a *fixed* total angular momentum (which is conserved), J and then minimise this energy with respect to J. This has two advantages. It reflects the quantum degeneracy of the lowest Landau level for electrons in a uniform magnetic field in the absence of any interaction, at the classical level itself and secondly it allows one to do the second step minimisation over the quantised values of the angular momentum. Here however we restrict ourselves to classical analysis only and derive some exact results analytically.

In particular we show that: a) the configurations minimising the energy are *independent* of the parameters of the Hamiltonian (eg magnetic field) so long as the repulsive two body potential falls off as a power-law (or vary logarithmically) with the relative distance. Only the overall length scale is sensitive to these details. 2) Two special configurations in which all the N particles are on a circle (referred to as ◯) and the one in which N - 1 are on a circle with one at the center (referred to as ⊙) are always (local) minimum energy configurations. We give exact analytical expressions for the corresponding minimum energy for all N. The ◯ has lower energy for $N \leq 5$ while ⊙ has lower energy for $N \geq 6$. This geometric transition is the first one to occur and is *independent* of the precise form of the repulsive interaction. 3) While it is known *numerically* that for $N \geq 9$ and for Coulomb potential [5,6] the minimum energy configurations exhibit approximate multi shell structure, the special configurations provide an upper bound on the minimum energy for a whole class of interactions that we consider here.

The classical system we are interested consists of N particles confined in an oscillator potential in a uniform magnetic field and interacting via a two body interaction. The Hamiltonian of such a system of particles given by,

$$H = \sum_{i=1}^{N} \left[\frac{(\vec{p}_i + \vec{a}_i)^2}{2m} + \frac{1}{2} m\omega^2 r_i^2 \right] + \beta \sum_{i,j(\neq i)} \frac{1}{(r_{ij}^2)^\nu}, \quad (1)$$

where $\vec{r}_i$ and $\vec{p}_i$ denote the position and momentum vectors of the i-th particle. The vector potential, for a uniform magnetic field is given by,

$$(a_i)_x = -\omega_L y_i \ \ ; \qquad (a_i)_y = \ \omega_L x_i, \quad (2)$$

where ω_L is the Larmor frequency and $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$. The power ν (positive) is kept arbitrary. In what follows we also comment on case when the two-body interaction is of the form $-\beta \sum_{i,j(\neq i)} \log(r_{ij}^2/\rho^2)$ which is repulsive for $r_{ij}^2 < \rho^2$. This may be closer to the real situation as also the $\nu = 1/2$ (Coulomb) in the case of electrons in a quantum dot [7]. Recently, the $\nu = 1$ case has also been analysed in detail [8]. The Hamiltonian can be written in terms of dimensionless units by introducing a length scale $l = \sqrt{(\hbar/(m\omega)}$ which is the basic oscillator length. All distances are measured in terms of this basic length unit. Note that the $\hbar$ is introduced only as a convenience so that the energy is measured in units of $\hbar\omega$ and does not have any other significance as in the quantum case. The momenta are measured in units of $\hbar/l$.

The new Hamiltonian in these scaled units, but keeping the same notation, may be written as

$$\frac{H}{\hbar\omega} = \sum_{i=1}^{N}\left[\frac{\vec{p_i}^{\,2}}{2} + \frac{1}{2}(1+\alpha^2)r_i^2 + \alpha j_i\right] + g\sum_{i,j(\neq i)}\frac{1}{(r_{ij}^2)^\nu}, \tag{3}$$

where $j_i = \vec{r}_i \times \vec{p}_i$, $\alpha = \frac{\omega_L}{\omega}$ and $g = \frac{\beta}{\hbar\omega}(l)^{2\nu}$. Unless otherwise mentioned the summations run from 1 to N hereafter. While the original coupling constant β was dimensional the new coupling constant g is dimensionless. Hereafter we assume all the energies are measured in units of $\hbar\omega$ and do not write the units explicitly.

For the first step of the minimisation we introduce the function,

$$F = H + \lambda(J - \sum_i j_i), \tag{4}$$

where j_i are the single particle angular momenta and λ is the Lagrange multiplier which enforces the constraint $J = \sum_i j_i$. Setting $\delta F = 0$, gives the necessary equations to determine the equilibrium configuration in the phase space,

$$p_{ix} = (\alpha+\lambda)y_i, \tag{5}$$

$$p_{iy} = -(\alpha+\lambda)x_i, \tag{6}$$

$$(1-\lambda^2-2\alpha\lambda)\vec{r}_i = 4g\nu\sum_{j(\neq i)}\frac{\vec{r}_{ij}}{(r_{ij}^2)^{\nu+1}}. \tag{7}$$

These are the basic set of equations. Any solution to this set of equations describes an equilibrium configuration but not necessarily the one with the minimum energy for the given J. The case of logarithmic interaction is obtained by simply setting the power $\nu = 0$ and by setting the prefactor to $4g$ instead of $4g\nu$ in eq.(7). With this proviso, unless otherwise mentioned, all subsequent equations also reproduce the log case.

First we present a qualitative but a general analysis of these basic set of equations. To make the analysis simple, we introduce an auxiliary variable,

$$\phi = \sum_i r_i^2. \tag{8}$$

The total angular momentum may now be written in terms of this auxiliary variable as

$$J = \sum_i \vec{r}_i \times \vec{p}_i = -(\alpha+\lambda)\phi, \tag{9}$$

where we have made use of eqs.(5,6). It is convenient to express $\vec{r}_i = R\vec{s}_i$ with R being a common scale factor which may be taken to be the radius of the farthest particle, say the N^{th} one. Therefore

$$\phi = R^2[\sum_{i=1}^{N-1} s_i^2 + 1] \equiv R^2\tilde{\phi} \tag{10}$$

since $s_N^2 = 1$. Using eq.(7) and eliminating λ dependence using eq.(9) we have,

$$\frac{(R^2)^{\nu+1}}{4g\nu}[1+\alpha^2-\frac{J^2}{R^4\tilde{\phi}^2}]\vec{s}_i = \sum_{j(\neq i)}\frac{\vec{s}_{ij}}{(s_{ij}^2)^{\nu+1}}. \tag{11}$$

Taking scalar product with $\vec{s}_i$ and dividing both sides by s_i^2 ($\neq 0$), we get,

$$\frac{(R^2)^{\nu+1}}{4g\nu}[1+\alpha^2-\frac{J^2}{R^4\tilde{\phi}^2}] = \sum_{j(\neq i)}\frac{1-(s_j/s_i)\cos(\theta_{ij})}{(s_i^2+s_j^2-2s_is_j\cos(\theta_{ij}))^{\nu+1}}. \tag{12}$$

Note that the LHS is independent of the particle index i. Thus we have $N-1$ independent of equations of the type

$$\sum_{j(\neq i)}\frac{1-(s_j/s_i)\cos(\theta_{ij})}{(s_i^2+s_j^2-2s_is_j\cos(\theta_{ij}))^{\nu+1}} = \sum_{j(\neq k)}\frac{1-(s_j/s_k)\cos(\theta_{kj})}{(s_k^2+s_j^2-2s_ks_j\cos(\theta_{kj}))^{\nu+1}}, \quad \forall \quad k \neq i. \tag{13}$$

Further by taking the cross product with $\vec{s}_i$ and dividing by s_i, we get,

$$\sum_{j(\neq i)}\frac{s_j\sin(\theta_{ij})}{(s_i^2+s_j^2-2s_is_j\cos(\theta_{ij}))^{\nu+1}} = 0, \tag{14}$$

which provides a further set of N conditions on the internal coordinates $\vec{s}_i$. Notice that these conditions are manifestly scale invariant. Together eqs.(13,14) provide the $2N-1$ necessary equations for determining the s_i and the angles θ_i. Notice that these determining equations are completely independent of α, J and g. We have therefore the result that $(s_1, s_2, ..., s_{N-1}, \theta_1, \theta_2, ..., \theta_N)$ are independent of the magnetic field (α), the total angular momentum J and the interaction strength g. These parameters, however, determine the overall scale R through eq.(12). In fact since $s_N^2 = 1$, the corresponding equation may be taken to be the determining equation for R in terms of the parameters of the Hamiltonian,

$$\frac{(R^2)^{\nu+1}}{4g\nu}[1+\alpha^2-\frac{J^2}{R^4\tilde{\phi}^2}] = \sum_{j=1}^{N-1}\frac{1-s_j\cos(\theta_{Nj})}{(1+s_j^2-2s_j\cos(\theta_{Nj}))^{\nu+1}} \equiv A(\nu,N) \tag{15}$$

Note that $A(\nu, N)$ introduced above is a function of ν and N only. Thus we have a *very general* result that the *geometry* or the shell structure of the equilibrium configuration is *independent* of the parameters of the Hamiltonian which only restrict the overall size of the system. The shell structure, however, depends on the nature of repulsive interaction through the parameter ν but not its

strength. The above analysis is valid even if any one of the $s_i = 0$, that is one particle being at the origin of the coordinate system in which case we have two equations less (not more than one particle can be at the origin).

The energy of the equilibrium configuration can be easily computed by noting that the auxiliary variable ϕ defined in eq.(8) is related to the two body potential energy by,

$$(1+\alpha^2-\frac{J^2}{\phi^2})\phi = 2g\nu \sum_{i,j(\neq i)} \frac{1}{(r_{ij}^2)^\nu}, \tag{16}$$

where the RHS is proportional to the potential energy due to interaction. Since the RHS and ϕ are positive definite we have the condition $(1+\alpha^2)\phi^2 > J^2$. Interestingly taking further gradients of the above equation again yield conditions on ϕ which violate the above inequality. Thus the minima described by the equations (5,6, 7) must be *isolated*. We have for the energy at the extrema,

$$\begin{aligned} E &= \frac{1}{2}[(1+\alpha^2)\phi + 2\alpha J + \frac{J^2}{\phi}] + g\sum_{i,j(\neq i)} \frac{1}{(r_{ij}^2)^\nu} \\ &= \frac{\nu+1}{2\nu}(1+\alpha^2)\phi + \alpha J + \frac{\nu-1}{2\nu}\frac{J^2}{\phi}, \end{aligned} \tag{17}$$

where $\phi = R^2\tilde{\phi}$ and $\tilde{\phi}$ is independent of J. This then is the energy of the equilibrium configuration in a given J sector. For the logarithmic case, the first line of eq.(17) has the second term corresponding to the logarithmic interaction and the second line is not valid.

In order to find the global minimum we now minimise the energy with respect to J and set $\partial E/\partial J = 0$, that is,

$$\begin{aligned} &[(\nu+1)(1+\alpha^2)R - (\nu-1)\frac{J^2}{\tilde{\phi}^2R^3}]\frac{\partial R}{\partial J} \\ &+ \frac{\nu\alpha}{\tilde{\phi}} + (\nu-1)\frac{J}{\tilde{\phi}^2R^2} = 0. \end{aligned} \tag{18}$$

Differentiating the R w.r.t. J in eq.(15) yields $\partial R/\partial J$ which when substituted in the above equation gives the J value and the corresponding global minimum energy,

$$J = -\alpha\tilde{\phi}R^2; \quad E = \frac{\nu+1}{2\nu}\tilde{\phi}R^2, \tag{19}$$

where

$$R^2 = [4g\nu A(\nu,N)]^{\frac{1}{\nu+1}}, \tag{20}$$

and $A(\nu,N)$ is defined before in eq.(15). An important point to note here is that the minimum energy E is *independent* of the magnetic field and its dependence on g is explicit. The dependence on N and ν is however involved. The angular momentum J at minimum of energy depends on the magnetic field and is zero in the absence of the magnetic field as it should be. The expressions given above, though, are valid independent of the geometry of the clusters and are exact (for approximate solutions see eqs.(8,9) in ref. [4] for the special case of Coulomb interaction).

The geometry of the clusters or shells are dependent on $\tilde{\phi}$ and $A(\nu,N)$ which are as yet unspecified. In general the equations for the equilibrium configurations admit many solutions (which are isolated as remarked earlier) for a given N and ν. In particular there are two special configurations which are always solutions viz (i) all the N particles are on a circle , $\bigcirc$ and (ii) $N-1$ particles are on the circle with one particle at the center, $\bigodot$. For these two cases only the over all scale factor R is to be determined. The angles, $\theta_{ij}/2$, are simply multiples of π/N and $\pi/(N-1)$ respectively. These however need not be minimum energy configurations for a given N and ν. In fact it has been numerically proved that for $N \leq 5$ the circle configuration is indeed the minimum energy configuration where as for $6 \leq N \leq 8$ it is the circle-dot which is the minimum energy configuration in the case of Coulomb interaction ($\nu = 1/2$). Multiple shells start forming for $N \geq 9$. In what follows we prove analytically that the first transition which occurs for N from 5 to 6 is independent of ν. The case of circle and circle-dot is particularly simple since there is only one scale involved. That is all $s_i^2 = 1, i = 2, ..., N$ and $s_1^2 = 1$ for the circle and $s_1^2 = 0$ for the circle-dot.

For the circle case, we have,

$$\tilde{\phi} = [\sum_{i=1}^{N-1} s_i^2 + 1] = N \tag{21}$$

and therefore the energy is given by,

$$E_\bigcirc = \frac{\nu+1}{2\nu}[4g\nu A_\bigcirc N^{\nu+1}]^{\frac{1}{\nu+1}}, \tag{22}$$

where

$$A_\bigcirc(\nu,N) = \frac{1}{2^{2\nu+1}}\sum_{k=1}^{N-1}\frac{1}{\sin^{2\nu}(\frac{k\pi}{N})}. \tag{23}$$

In the case of circle-dot, we have,

$$\tilde{\phi} = N-1 \tag{24}$$

since there are now $N-1$ particles on the circle and therefore the energy is given by,

$$E_\bigodot = \frac{\nu+1}{2\nu}[4g\nu A_\bigodot (N-1)^{\nu+1}]^{\frac{1}{\nu+1}}, \tag{25}$$

where

$$A_\bigodot(\nu,N) = A_\bigcirc(\nu,N-1) + 1. \tag{26}$$

The extra 1 on the RHS is due to the contribution of the particle at the center. To ascertain which of these two

configurations ◯ and ⊙ has lower energy it is sufficient to look at the ratio,

$$(\frac{E_{\bigcirc}}{E_{\bigodot}})^{\nu+1} \equiv f(\nu,N) = (\frac{N}{N-1})^{\nu+1} \frac{\lambda_N^{(\nu)}}{\lambda_{N-1}^{(\nu)} + 2^{2\nu+1}}, \quad (27)$$

where,

$$\lambda_N^{(\nu)} \equiv \sum_{k=1}^{N-1} \frac{1}{\sin^{2\nu}(\frac{k\pi}{N})}. \quad (28)$$

Note that in general the ratio f depends only on N and ν. Obviously the circle is a lower energy configuration iff $f < 1$. We claim that, for all $\nu > 0$,

$$\begin{array}{lll} f(\nu,N) & < & 1 \quad \text{for} \quad N \leq 5; \\ f(\nu,N) & > & 1 \quad \text{for} \quad N \geq 6. \end{array} \quad (29)$$

Further the function $f(\nu,N)$ crosses unity exactly once for N between 5 and 6 and nowhere else. This result can be easily seen for $\nu = 1$ since in this case $\lambda_N^{(1)} = (N^2-1)/3$. Therefore,

$$f(1,N) = \frac{N^2(N+1)}{(N-1)(N^2-2N+24)} \quad (30)$$

which reproduces the claims made above, for $\nu = 1$. The general proof of these claims for *all* ν is some what involved and will be published elsewhere. We sketch the arguments for the case $\nu << 1$, where one may use the expansion $a^\nu \approx 1 + \nu \log(a)$. Using this λ_N may be written as,

$$\lambda_N^{(\nu)} \approx N - 1 - 2\nu X_N, \quad (31)$$

where

$$X_N = \log[\prod_{k=1}^{N-1} \sin(\frac{k\pi}{N})] = \log[\frac{N}{2^{N-1}}], \quad (32)$$

where we have used the identity $\prod_{k=1}^{N-1} \sin(\frac{k\pi}{N}) = \frac{N}{2^{N-1}}$. Substituting for λ_N in f, we have

$$f(\nu,N) \approx 1 + \frac{\nu}{N(N-1)} \mu_N, \quad (33)$$

where

$$\mu_N = [N(N-3)\log(N) - (N-1)(N-2)\log(N-1)]. \quad (34)$$

is independent of ν. It is now easy to see that μ_N is negative for $N \leq 5$ and positive otherwise. Hence the claim. In the case of logarithmic interaction, the transition can be seen more easily by taking the difference of energies for circle and circle-dot since this difference is independent of the arbitrary scale ρ in the interaction. It turns out that the difference is precisely given by $g\mu_N$. Therefore the first geometric transition also occurs for the log case exactly as in the power-law case.

To summarize, we have proved in general that the organisation of many body clusters in two dimensions into shells is a robust phenomenon independent of the nature of the repulsive two-body interaction and also independent of the Hamiltonian parameters but dependent only on the number of particles in the cluster. In particular we have analytically proved that the first geometric transition for the ground state from circle to circle-dot configuration occurs after $N = 5$. The robustness of this transition seems to emerge purely from the number theoretic properties of the ratios of the energies (difference in the log case) in these two configurations. It is an open question if this is due to some hidden symmetry properties. We have also done numerical simulations for larger N and for various values of ν. We find that the shell structure found by Bedanov and Peeters [5] in the case of Coulomb interaction is valid for all ν in general except that for larger ν the shell description is valid only approximately. The equilibrium configurations correspond to isolated minima. This fact should be useful in calculating quantum fluctuations about the minima. The details of these investigations will be published elsewhere.

We thank R. Balasubramanian and D. Surya Ramana for help with number theoretic identities. We also thank Madan Rao and Surajit Sengupta for helpful discussions and for a critical reading of the manuscript.

[1] For a detailed account of these developments, see for example, T. Chakraborty and P. Pietilainen, *The Quantum Hall Effects*, (Springer-Verlag, Heidelberg, 1995).

[2] R. Calinon, Ph. Choquard, E. Jamin and M. Navet, in *Ordering in two dimensions*, ed. S. K. Sinha (Elsevier, New York, 1980)p.317.

[3] Yu. E. Lozovik and V. A. Mandelshtam, Phys. Lett. **A145**, 269(1990); Phys. Lett. **A165**,469(1992).

[4] P. A. Maksym, Phys. Rev. **B53**, 10871(1996).

[5] V. M. Bedanov and F. M. Peeters, Phys. Rev. **B49**, 2667(1994).

[6] F. Bolten and U. Rossler, Superlatt. and Microstruct. **13**, 140(1993).

[7] F. C. Zhang and S. Das Sarma, Phys. Rev. **B33**, 2903(1986).

[8] N. F. Johnson and L. Quiroga, Phys. Rev. Lett. **74**, 4277(1995); see also Preprint - cond-mat/9610224 (1996) for a detailed study of inverse square interaction.